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First principles and atomistic calculations of Mg segregation in Al grain-boundaries

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Al-Mg alloys with higher Mg contents are highly desirable due to their higher tensile and fatigue strength and better weldability. However, higher Mg concentration (more than 6 wt%) leads to reduced hot workability and more stress corrosion cracking. There are several experimental indications that the hot-working edge fracture might be due to Mg segregation to the grain-boundaries (GBs). The Monte-Carlo simulations using force-matching embedded-atom method (EAM) potentials confirm the Mg enrichment at the GB surfaces. To verify the validity of the Monte-Carlo results and the EAM potentials, we have carried out a series of ab-initio electronic structure calculations of Mg doped in various types of Al GBs. The ab-initio calculations were performed based on the pseudopotential method and the local density functional theory. The results for Mg segregation enthalpy and bonding characteristics in Al GBs will be presented.

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